

On thermodynamic consistency of strain gradient elasticity

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Abstract

Thermodynamic consistency assures that a description of a phenomenon satisfies the fundamental laws of thermodynamics. Verifying thermodynamic consistency of strain gradient elasticity is not trivial. It involves introducing internal variables. The single internal variable theory provides a framework for justifying the thermodynamic consistency of strain gradient elasticity. The dual internal variables approach, which produces hyperbolic evolution equations, overcomes the restrictions of strain gradient elasticity models.

Keywords: strain gradient elasticity, thermodynamic consistency, internal variables

1 Introduction

Classical elasticity theory holds true for homogeneous solids. To characterize the behavior of inhomogeneous or microstructured materials, a more general framework is necessary. The strain gradient elasticity is the first choice for enhancing the classical theory of elasticity.

A recent review (Desai and Sidhardh 2025) outlines the current state-of-the-art in strain gradient elasticity. It is remarkable that this review just discusses strain gradient models with mechanical origins. This reflects the historical path of the development of strain gradient models. Following pure mechanical seminal works by Mindlin (1964); Mindlin and Eshel (1968), numerous papers created reduced versions of the strain gradient elasticity (Lam et al. 2003; Papargyri-Beskou et al. 2009; Papanicolopoulos and Zervos 2010; Askes and Aifantis 2011; Zhou et al. 2016; Eremeyev and Dell’Isola 2018; Fu et al. 2020, e.g.). Simplified strain gradient models (Aifantis 1999; Askes and

Aifantis 2006; Askes et al. 2008; Aifantis 2020) also skip thermodynamic considerations. Discrete lattice based strain gradient models (Metrikine and Askes 2002; Askes and Metrikine 2005; Askes et al. 2008; DeDomenico et al. 2019; Andrianov et al. 2022) have no reference to thermodynamics by definition.

Thermodynamic consistency is of great importance in strain gradient theories because it keeps models in accordance with fundamental physical laws (Papenfuss and Forest 2006). It has been shown that Mindlin-type strain gradient models are compatible with thermodynamics when an energy transfer equation is assumed in addition to the conventional energy balance law (Broese et al. 2016; Alber et al. 2018). At the same time, thermodynamic features of the strain gradient elasticity are missing in the recently published book (Bertram and Forest 2020).

Checking the thermodynamic consistency of strain gradient elasticity is not straightforward, as exemplified by a simple one-dimensional example in section 3. The verification can be achieved as a consequence of the analysis of the single internal variable model in Section 4. The corresponding evolution equation for the internal variable is not hyperbolic, and the resulting equation of motion has a lack of causality (Metrikine 2006). The hyperbolicity of the internal variable equations is recovered in Section 5 using the dual internal variables approach. The thermodynamic aspects are examined in a one-dimensional setting.

2 One dimensional strain gradient elasticity

2.1 One-dimensional linear elasticity

In the small strain approximation, elastic behavior of materials is governed by the Hooke law, which in one-dimensional settings can be expressed as

$$\sigma = \rho c^2 u_x, \quad (1)$$

where σ is the Cauchy stress, ρ is the matter density, c is the wave speed, u is the displacement, and subscript denotes the derivative. The corresponding free energy per unit volume is the following:

$$W = \frac{\rho c^2}{2} u_x^2. \quad (2)$$

Using the balance of linear momentum in the absence of body forces

$$\rho u_{tt} = \sigma_x, \quad (3)$$

we arrive at the classical wave equation

$$u_{tt} = c^2 u_{xx}. \quad (4)$$

2.2 Strain gradient model

According to the one-dimensional strain gradient model, the free energy per unit volume depends on both the strain $\varepsilon = u_x$ and its gradient u_{xx} . Keeping the quadratic

relationship for the free energy, we get

$$W = \frac{\rho c^2}{2} u_x^2 + A u_x u_{xx} + \frac{1}{2} B u_{xx}^2, \quad (5)$$

where A and B are material parameters. Equation (5) is the simplest quadratic form that includes both strain and its gradient. Due to the symmetry constraints, coefficient A should vanish (dell'Isola et al. 2009). The symmetric form of the free energy dependence is

$$W = \frac{\rho c^2}{2} u_x^2 + \frac{1}{2} B u_{xx}^2. \quad (6)$$

The associated stresses are specified as follows:

$$\sigma = \frac{\partial W}{\partial u_x} = \rho c^2 u_x, \quad \tau = \frac{\partial W}{\partial u_{xx}} = B u_{xx}. \quad (7)$$

The equation of motion is expressed as (Mindlin and Eshel 1968)

$$\rho u_{tt} = \sigma_x - \tau_{xx} = \rho c^2 u_{xx} - B u_{xxxx}. \quad (8)$$

3 Thermodynamic consistency

We now examine the thermodynamic consistency of the one-dimensional strain gradient elasticity model. The thermodynamic extension of the model incorporates temperature θ as a state variable. Therefore, the free energy per unit volume is represented as

$$W = W(u_x, \theta, u_{xx}). \quad (9)$$

One-dimensional motion in thermoelastic heat conductors is governed by the local balance law for energy in addition to that for the linear momentum

$$\left(\frac{\rho v^2}{2} + E \right)_t - (\sigma v - Q)_x = 0, \quad (10)$$

and by the second law of thermodynamics

$$S_t + \left(\frac{Q}{\theta} \right)_x \geq 0. \quad (11)$$

Here $v = u_t$ is the particle velocity, E is the internal energy per unit volume, S is the entropy per unit volume, Q is the heat flux.

Since the internal energy is related to the free energy $E = W + \theta S$, we have

$$\rho v v_t + (W + \theta S)_t - (\sigma v - Q)_x = 0. \quad (12)$$

Due to the balance of linear momentum

$$\rho v_t = \sigma_x, \quad (13)$$

and the time derivative of the free energy

$$W_t = \frac{\partial W}{\partial u_x} u_{xt} + \frac{\partial W}{\partial \theta} \theta_t + \frac{\partial W}{\partial u_{xx}} u_{xxt} = \sigma v_x - S\theta_t + \tau u_{xxt}, \quad (14)$$

the energy balance can be represented as

$$-S\theta_t + \tau u_{xxt} + (\theta S)_t + Q_x = 0. \quad (15)$$

We may reformulate the second law as the Clausius-Duhem inequality by multiplying it by temperature and applying the energy balance

$$\tau u_{xxt} - \frac{Q}{\theta} \theta_x \geq 0. \quad (16)$$

In the isothermal case, inequality (16) reduces to

$$\tau u_{xxt} \geq 0. \quad (17)$$

In the non-dissipative case, we have then

$$\tau u_{xxt} = 0. \quad (18)$$

Since τ is the derivative of free energy with respect to the strain gradient, it is determined by the specification of the free energy function. As a result, thermodynamic consistency in the non-dissipative case requires time-independence for the strain gradient. This is an extremely restrictive condition. We shall have to examine the situation in a broader context.

4 Single internal variable

The extension of the state space of linear thermoelasticity by the strain gradient can be generalized using internal variable theory. Strain gradient elasticity with internal variables has been discussed by Papenfuss and Forest (2006) resulting in the choice of the possible state space. Another viewpoint was offered in (Ván 2020), where internal variables were introduced in addition to the strain gradient. Our approach accounts the influence of the microstructure on macroscopic behavior by introducing an internal variable α that represents the integral distributed effect of the microstructure (Berezovski and Ván 2017)(Sect.3.4). The free energy W is specified as a sufficiently regular function of strain, temperature, the internal variable α , and its space derivative

$$W = W(u_x, \theta, \alpha, \alpha_x). \quad (19)$$

The corresponding equations of state are given by (Maugin and Muschik 1994)

$$\sigma := \frac{\partial W}{\partial u_x}, \quad S := -\frac{\partial W}{\partial \theta}, \quad \tau := -\frac{\partial W}{\partial \alpha}, \quad \eta := -\frac{\partial W}{\partial \alpha_x}. \quad (20)$$

In terms of free energy, the energy balance is

$$(W + \theta S)_t - \sigma v_x + Q_x = 0. \quad (21)$$

Time derivative of free energy is determined using the chain rule

$$W_t = \frac{\partial W}{\partial u_x} u_{xt} + \frac{\partial W}{\partial \theta} \theta_t + \frac{\partial W}{\partial \alpha} \alpha_t + \frac{\partial W}{\partial \alpha_x} \alpha_{xt} = \sigma v_x - S \theta_t - \tau \alpha_t - \eta \alpha_{xt}, \quad (22)$$

which reduces the energy balance (21) to

$$-S \theta_t - \tau \alpha_t - \eta \alpha_{xt} + (\theta S)_t + Q_x = 0. \quad (23)$$

The second law incorporates the extra entropy term K (Müller 1967; Maugin 1990, 2006). By multiplying the second law by temperature

$$\theta S_t + \theta \left(\frac{Q}{\theta} + K \right)_x \geq 0. \quad (24)$$

and accounting for the energy balance, we get the Clausius-Duhem inequality

$$\tau \alpha_t + \eta \alpha_{xt} - \left(\frac{Q}{\theta} + K \right) \theta_x + (\theta K)_x \geq 0. \quad (25)$$

The dissipation inequality (25) can be rearranged as

$$(\tau - \eta_x) \alpha_t - \left(\frac{Q}{\theta} + K \right) \theta_x + (\eta \alpha_t + \theta K)_x \geq 0. \quad (26)$$

The non-zero extra entropy flux K is selected following (Maugin 1990) in the form

$$K = -\theta^{-1} \eta \alpha_t. \quad (27)$$

This choice allows us to reduce the dissipation inequality to

$$(\tau - \eta_x) \alpha_t - \left(\frac{Q - \eta \alpha_t}{\theta} \right) \theta_x \geq 0. \quad (28)$$

In this case, dissipation is clearly separated into intrinsic and thermal parts. This implies that the dissipation inequality in the isothermal case reduces to

$$(\tau - \eta_x) \alpha_t \geq 0. \quad (29)$$

The evolution equation for the internal variable is selected to ensure that the dissipation inequality is satisfied

$$\alpha_t = R(\tau - \eta_x), \quad (30)$$

where R is a positive coefficient.

In the nondissipative case, the evolution equation for internal variable can be expressed in the form

$$(\tau - \eta_x) = 0. \quad (31)$$

To be more specific, we represent the free energy as a quadratic function

$$W = \frac{\rho c^2}{2} u_x^2 + A \alpha_x u_x + \frac{1}{2} B \alpha^2 + \frac{1}{2} C \alpha_x^2, \quad (32)$$

It follows from equations of state (20) that

$$\sigma = \frac{\partial W}{\partial u_x} = \rho c^2 u_x + A \alpha_x, \quad \tau = -\frac{\partial W}{\partial \alpha} = -B \alpha, \quad \eta = -\frac{\partial W}{\partial \alpha_x} = -A u_x - C \alpha_x, \quad (33)$$

and evolution equation is an equation of reaction-diffusion type

$$\frac{1}{R} \alpha_t = C \alpha_{xx} + A u_{xx} - B \alpha. \quad (34)$$

In the non-dissipative case (when $\alpha_t = 0$)

$$C \alpha_{xx} + A u_{xx} - B \alpha = 0, \quad (35)$$

and the balance of linear momentum (3) can be represented in terms of the displacement as

$$\rho u_{tt} = \rho c^2 u_{xx} + A \alpha_{xx} = \rho c^2 u_{xx} + \frac{C}{B} (\rho u_{tt} - \rho c^2 u_{xx})_{xx} + \frac{A^2}{B} u_{xxxx}. \quad (36)$$

If the quadratic nonlocality term can be neglected ($C = 0$), then we get

$$B \alpha = A u_{xx}, \quad (37)$$

and the internal variable is proportional to the strain gradient. In this case, the equation of motion (36) is reduced to that of the strain gradient elasticity

$$\rho u_{tt} = \rho c^2 u_{xx} + \frac{A^2}{B} u_{xxxx}. \quad (38)$$

This justifies the thermodynamic consistency of the strain gradient elasticity model in one dimensional setting. Although the equations of motion (8) and (38) are similar, they were obtained using different approaches. The thermodynamically consistent equation (38) is derived from the free energy in the form

$$W = \frac{\rho c^2}{2} u_x^2 + A (u_{xx})_x u_x + \frac{1}{2} B u_{xx}^2, \quad (39)$$

which is compatible with Aifantis-type strain gradient model (Aifantis 1999; Askes and Aifantis 2006)

$$\sigma = \rho c^2 u_x + A(u_x)_{xx}. \quad (40)$$

The evolution equation for the internal variable (34) describes relaxation to equilibrium (Ván 2020). This means that the single internal variable theory does not capture the inner dynamics. To find the solution to this issue, we will employ the dual internal variable approach (Ván et al. 2008),(Berezovski and Ván 2017)(Sect.4.2).

5 Dual internal variables

In the dual internal variables approach, it is suggested that an extra internal variable, say β , should be introduced to reflect a more broad class of phenomena (Berezovski and Ván 2017)(Sect.4.2). In the most basic situation, the functional form of free energy per unit volume includes the quadratic contribution of β

$$W = \frac{\rho c^2}{2} u_x^2 + A \alpha_x u_x + \frac{1}{2} B \alpha^2 + \frac{1}{2} C \alpha_x^2 + \frac{1}{2} D \beta^2. \quad (41)$$

Extending the state space results in dual evolution equations for internal variables. In the non-dissipative case, the primary internal variable is governed by the secondary one, and vice versa (Berezovski and Ván 2017)(Sect.6.6)

$$\alpha_t = -D\beta, \quad \beta_t = -(C\alpha_{xx} + Au_{xx} - B\alpha). \quad (42)$$

It is apparent that the secondary internal variable can be eliminated to get the single evolution equation for the internal variable α

$$\alpha_{tt} = -D\beta_t = D(C\alpha_{xx} + Au_{xx} - B\alpha). \quad (43)$$

The evolution equation (43) and the balance of linear momentum

$$\rho u_{tt} = \rho c^2 u_{xx} + A\alpha_{xx}, \quad (44)$$

form a coupled system of equations.

5.1 Hyperbolicity

The system of second order equations can be expressed as a first order system of equations. Introducing the variable w such that

$$u_t = w_x, \quad (45)$$

we can rewrite the balance of linear momentum as

$$\rho w_t = \rho c^2 u_x + A\alpha_x. \quad (46)$$

Similarly, the variable ϕ such that

$$\alpha_t = \phi_x, \quad (47)$$

allows to reduce the order of the evolution equation

$$\phi_t = DC\alpha_x + DAu_x - D \int B\alpha dx. \quad (48)$$

To check the hyperbolicity, the obtained first order system of equations can be represented in the matrix form

$$\frac{d}{dt} \begin{pmatrix} u \\ w \\ \alpha \\ \phi \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ c^2 & 0 & A/\rho & 0 \\ 0 & 0 & 0 & 1 \\ AD & 0 & CD & 0 \end{pmatrix} \frac{d}{dx} \begin{pmatrix} u \\ w \\ \alpha \\ \phi \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ -BD \int \alpha dx \end{pmatrix}. \quad (49)$$

Characteristic polynomial of this system of equations

$$\det \begin{pmatrix} -\lambda & 1 & 0 & 0 \\ c^2 & -\lambda & A/\rho & 0 \\ 0 & 0 & -\lambda & 1 \\ AD & 0 & CD & -\lambda \end{pmatrix} = \lambda^4 - CD\lambda^2 - c^2\lambda^2 + CDc^2 - \frac{A^2D}{\rho}, \quad (50)$$

has real roots

$$\lambda^2 = \frac{1}{2}(c^2 + CD) \pm \sqrt{\frac{(c^2 - CD)^2}{4} + \frac{A^2D}{\rho}}, \quad (51)$$

which confirms the strict hyperbolicity of the system of equations. The eigenvalues λ^2 represent square of finite wave speeds. If there is no coupling between strain and internal variable (i.e., $A = 0$) than

$$\lambda^2 = \frac{1}{2}(c^2 + CD) \pm \frac{1}{2}(c^2 - CD). \quad (52)$$

This means that in addition to the velocity of elastic wave c there is an additional wave speed \sqrt{CD} characterizing motion of microstructure. In the case of coupling, both velocities are affected by A^2D/ρ .

The equation of motion in terms of displacement

$$(\rho u_{tt} - \rho c^2 u_{xx})_{tt} = DC(\rho u_{tt} - \rho c^2 u_{xx})_{xx} + A^2 D u_{xxxx} - BD(\rho u_{tt} - \rho c^2 u_{xx}), \quad (53)$$

has no problems with causality (Berezovski 2022).

6 Conclusions

Strain gradient elasticity models are used to describe a variety of problems (Lam et al. 2003; Askes and Aifantis 2011) because they capture size effects (Aifantis 1999).

The strain gradient approach has known limitations, including questionable boundary conditions for higher-order derivatives (Askes and Metrikine 2005; Askes et al. 2008), accounting only for the acoustic branch of the dispersion curve (Papargyri-Beskou et al. 2009; DeDomenico and Askes 2016), and the inability to avoid causality issues (Metrikine 2006).

Thermodynamic consistency of strain gradient elasticity is frequently overlooked in favor of variational techniques. To verify the thermodynamic consistency of the strain gradient elasticity, the thermodynamic framework with internal variables is adopted, guaranteeing that the second law is obeyed by construction (Berezovski and Ván 2017)(Sect.4.5). The time evolution of internal variables satisfies the Clausius-Duhem inequality.

As it is shown, single internal variable theory can justify the thermodynamic consistency of the strain gradient elasticity model but cannot improve their limitations. Only dual internal variables concept resulting in hyperbolic evolution equations for internal variables provides the motion of waves at finite speeds (respecting causality), accounts for both acoustic and optical branches of dispersion curve (Berezovski 2022), and simplifies boundary conditions. It captures inner dynamics in microstructured solids when coupled with macroscopic motion. Dual internal variables cannot be explicitly interpreted in terms of strain gradients, but they can be related with microdeformations in Mindlin microelasticity, which is the basis of strain gradient theories (Berezovski et al. 2011),(Berezovski and Ván 2017)(Sect.7.1).

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